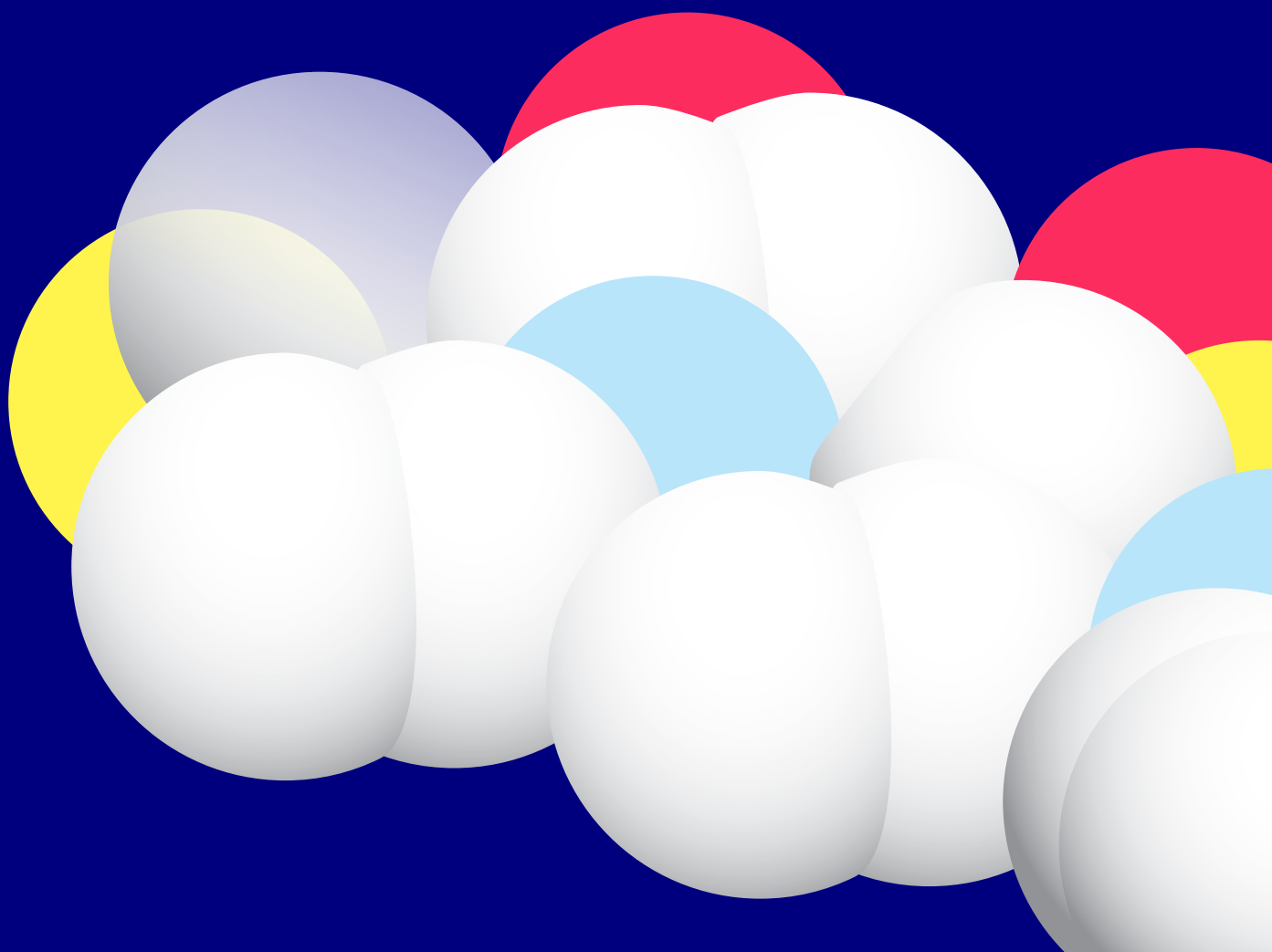


Solving the challenge of Chapter 29

Automated HS coding for organic chemicals



Solving the challenge of Chapter 29: Automated HS coding for organic chemicals

Every day, millions of tonnes of organic chemicals are bought, sold, distributed and delivered across the world – a process that’s regulated by Chapter 29 of the World Customs Organization (WCO) Harmonized System (HS).

Each of the vast number of chemical compounds needs an appropriate HS code before it’s traded and transported. A HS code is essential for calculating tax and duty for any chemical or commodity that crosses borders.

Obtaining the right HS code is critical to compliance but, too often, the responsibility for navigating this complex and highly-detailed guidance is given to those with limited scientific knowledge. This can lead to avoidable errors in coding that can cost businesses tens of thousands of dollars in unnecessary taxes every year.

In this white paper, we discuss the challenges of tariff-coding organic chemicals and present ExpediChem, a new cloud-based platform which enables non-chemists to generate accurate HS codes and duty calculations for common and novel/proprietary organic chemicals in seconds.

With ExpediChem, scientists and non-scientists can rapidly identify the correct HS code, reducing delays, saving money and increasing regulatory compliance – solving the challenge of Chapter 29.



“A simple, intuitive way to allow non-chemists to correctly HS code chemicals, reducing delays, saving money and increasing regulatory compliance”





What is Chapter 29?

The global trade in organic chemicals is massive. A European Union report found that organic chemicals represent 3% (by value) of all imports into the EU, representing billions of dollars worth of trade and taxes.¹

The international market for chemicals and compounds is regulated by the World Customs Organization (WCO) Harmonized System (HS). The extensive guidelines have been designed to standardise and simplify cross-border trade in goods and chemicals. Of all the chapters and commodity types covered by the Harmonized System, Chapter 29 (organic chemicals) is widely considered to be the hardest to follow, and the most difficult to apply. Chapter 29 is extensive, running to hundreds of pages. It's further complicated by extensive explanatory notes that must also be considered and understood.

The challenge of finding the right HS code doesn't stop there. Both the Pharmaceutical Appendix and the US-specific Chemical Appendix can alter the HS code or rates of duty to be declared, making the process more costly, complicated and time-consuming for businesses.



“In the USA implementation of the harmonized system (HTSUS), organic chemicals are covered by over 170 pages of complex rules relating to chemical structures and classes”

The challenge of coding chemicals

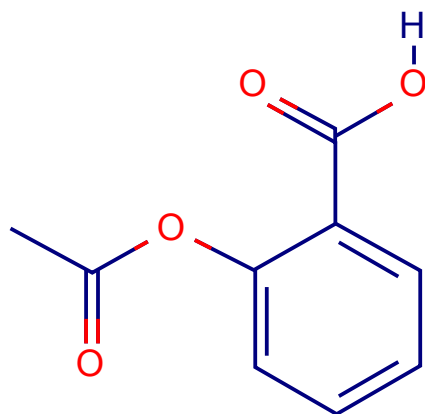
Identifying the correct HS code requires a comprehensive knowledge of chemistry and an in-depth knowledge of the rules, regulations and permutations of Chapter 29.

In the simplest of cases, you may have a CAS RN® (Chemical Abstracts Service Registry Number), that you can use in one of the available lookup systems, such as ECICS in the EU.²

However, such systems only cover a tiny percentage of traded chemicals. ECICS itself contains approximately 35,000 chemicals and 48,000 CAS RNs, but tens of millions of commercially available chemicals are traded worldwide. The Available Chemicals Directory alone lists over 11.7 million chemicals for sale.

Even if you are lucky enough to be shipping a common chemical, classification can still be difficult. A single chemical structure can be known by hundreds of different names, numbers and identifiers, but only cited as one or two names/identifiers in Chapter 29.

Take the chemical structure below:



This is the chemical structure for aspirin. Its Pubchem record lists over 400 different names, including aspirin, acetylsalicylic acid, 50-78-2, 2-Acetoxybenzoic acid, 2-(Acetyloxy)benzoic acid, O-Acetylsalicylic acid and o-Acetoxybenzoic acid.³

If you search for it using CAS number 50-78-2 in the HTSUS Chapter 29, you won't find it. Only two, of the 400 names aspirin is known by, are listed in the HTSUS.

If you've developed a new or proprietary chemical, it's your responsibility to determine the most applicable HS code and duty. Typically, chemicals are manually coded in-house against the complex chemical rules of Chapter 29 to determine the appropriate designation – a process that is prone to error.

Manually coding a new chemical is labour intensive and should only be completed by qualified and experienced chemists. External consultants can be used, but costs can quickly stack up.

Trade compliance lawyers or other specialists can charge between \$200 and \$800 per hour. Identifying the appropriate HS code for a single chemical is typically set at 1 – 2 hours of work and can take a few days to turn around. If you're shipping multiple chemicals or proprietary compounds at the same time, costs can rapidly increase.

If you're willing to wait for a result, you can disclose the structure to an official customs lab or authority for a determination.⁴ The process can take weeks or even months, leaving you with no option but to pause what you're doing until a HS code is delivered.

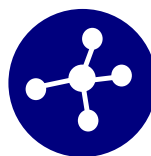
But there is an alternative. ExpediChem is a highly accurate and completely automated system that can determine the HS code for any organic chemical covered in Chapter 29 of the HTSUS (US import), Schedule B (US export), the EU and China. Created by scientists for non-scientists, it's a simple-to-use online platform designed specifically to tackle the challenge of Chapter 29.

“

“Easily HS-code chemicals in seconds, even novel and proprietary ones”

The solution: Searching with the structure

The limitations of searching for a chemical by name alone are widely understood and acknowledged. It's now common practice to perform chemically enabled searches, where you search for the molecular structure of a chemical against databases or rule sets.



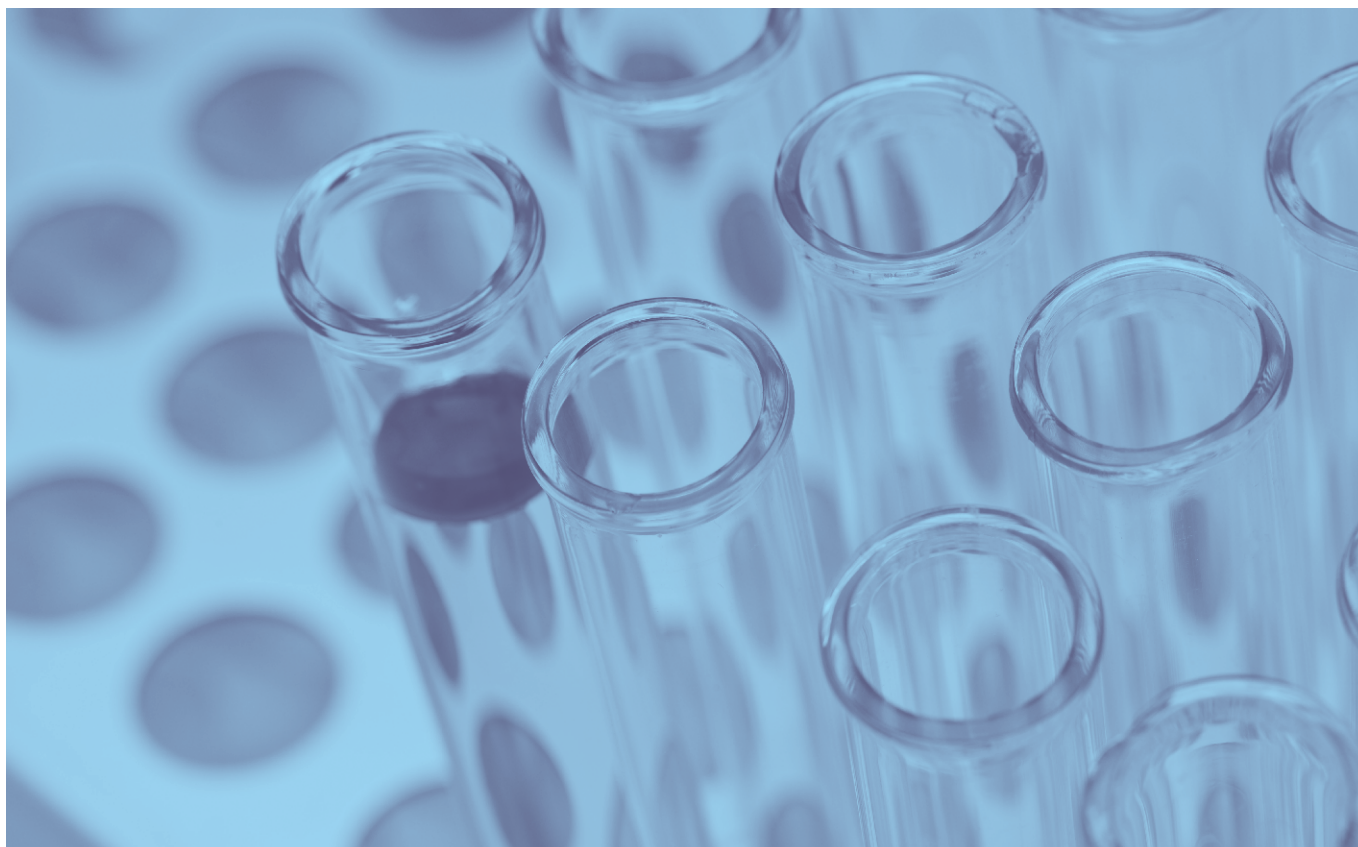
ExpediChem enables users to determine the HS code using the structure of a molecule. The system automatically applies the rules of Chapter 29 (including the named substances and various appendices, including the Pharmaceutical Appendix) with incredible accuracy.



The cloud-based platform can process hundreds of chemicals a minute, generating highly accurate HS codes and duty determinations for the US, EU and China.



In tests, ExpediChem is faster, more accurate and cheaper than highly trained and experienced chemists.

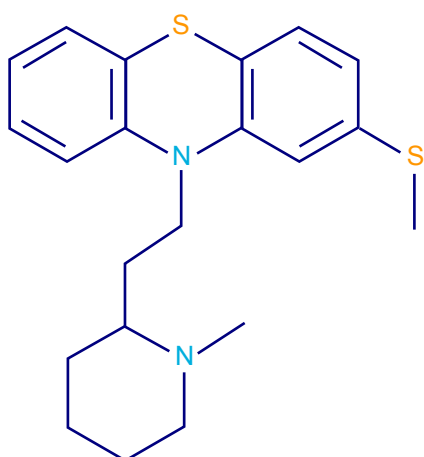




Capturing context

An additional complexity of Chapter 29 is that results can be context-sensitive. For example, the HS code and duty can vary for the same structure depending on how it will be used, or even its biological activity.

Take the structure below:



This is thioridazine, an antipsychotic drug. Its HTSUS code, based purely on structure, is 2934.30.5000. However, since it shows drug-like activity – specifically central nervous system activity in the brain – there is a more appropriate code. It is impossible to derive the potential use or activity solely from a chemical structure. Instead, to arrive at the most accurate HS code determination, contextual information can also be provided and considered.

When using the ExpediChem platform, users are prompted for additional information where relevant. They're given a range of possible options to choose from to support the HS code designation process. If the user is not aware of any additional information, they can leave the section blank, and a HS code and appropriate duty

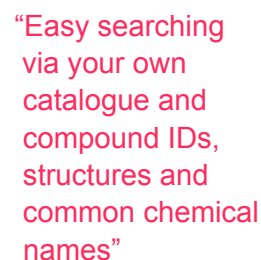
is calculated solely based on the chemical structure provided.

When context-specific information is provided, ExpediChem uses this to generate a more accurate HS code. In this case, ExpediChem has identified the most accurate HS code of 2934.30.2300 of the HTSUS (Drugs/Antidepressants, tranquilizers and other psychotherapeutic agents). While both results return the same 6-digit harmonized code, the extra context allows ExpediChem to arrive at a much more relevant 10-digit code.

In many cases, those tasked with obtaining HS codes work within trade compliance or shipping groups and have limited chemical knowledge.

ExpediChem allows you to paste in or upload common chemical text-based formats such as SMILES and InChI strings, or utilise formats such as .mol and .sd to upload chemicals to check, even proprietary or novel ones. You can also use the chemical sketching tool to draw molecules, allowing proprietary chemicals to be assigned appropriate HS codes and duties.

We continue to invest in innovation, and in the future, we hope to allow users to directly upload images that have been cut and pasted from other sources, such as websites. ExpediChem will use image recognition to calculate the HS code automatically. You can search for a chemical compound by name and retrieve its chemical structure, its HS code and duty calculation in seconds.



Scitegrity

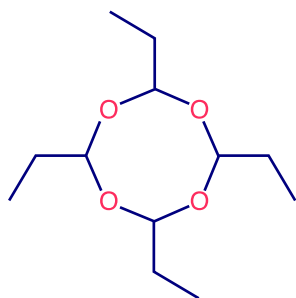
Accuracy and speed

Identifying the correct HS code is critical, with an incorrect code potentially costing you tens of thousands of dollars in unnecessary duty payments.

ExpediChem is quick, and there are no compromises on accuracy. For example, where Chapter 29 specifies that all salts, ethers or esters of a product are to be considered, they are. The platform can also discriminate between different stereo forms of molecules when appropriate.

In addition to Chapter 29, there is a related chemicals chapter: Chapter 28 (inorganic chemicals). While ExpediChem does not currently cover Chapter 28, it will refuse any attempts to force inorganic molecules into Chapter 29. Instead, you will be advised that other chapters are more suitable for the specific chemical structure. The ExpediChem system also accounts for extra chapter notes and explanatory notes, which can sometimes use definitions which may be counterintuitive to a trained chemist.

Take this example:



Initially, this appears to be O-heterocycle but is not classified here. If we refer to Chapter 29, Note 7, this compound is classified as a cyclic polymer of an aldehyde.

Chapter 29, note 7 states:

“Headings 2932, 2933 and 2934 do not include epoxides with a three-membered ring, ketone peroxides, cyclic polymers of aldehydes or of thioaldehydes, anhydrides of polybasic carboxylic acids, cyclic esters of polyhydric alcohols or phenols with polybasic acids, or imides of polybasic acids. These provisions apply only when the ring-position hetero-atoms are those resulting solely from the cyclizing function or functions here listed.”

Even for a HS-trained chemist with years of experience, this complexity would be easy to miss. ExpediChem can manage this, achieving impressive levels of accuracy with the most challenging chemical compounds.

To test and validate the system, we processed a test-set of structures from the European Customs Inventory for Chemical Substances (ECICS), a publicly available database of manually assigned HS/CN numbers from the EU Taxation and Customs Directorate General.

During our tests, ExpediChem achieved 99% accuracy in generating HS codes against 14,055 chemicals in headings 2901-2935 inclusive (8-digit level comparison). Where there were differences, ExpediChem correctly classified chemicals more effectively than the ECICS.



“During tests, ExpediChem achieved 99% accuracy in generating HS codes against 14,055 chemicals previously coded by EU customs authorities”

Mode of operation: Bulk

Number of Input Substances = 1

Number of Unreadable Input Substances = 0

Excel, PDF and SDF result files:

Return to start

Generate Excel results file

Generate PDF report

Download SDF results file

Tariff Information (all selected schedules): US_HTS, US_ScheduleB, EU_HS, CN_HS

Number of Readable Input Substances = 1

Number of Matched Substances = 1

Detailed HTS, US (US_Import)

Detailed US ScheduleB (US_Export)

Detailed EU

Detailed Chinese (PNC)

Detailed USHTS (US Import) results

Identifier	Input Molecule	USHTS Code (US Import)	USHTS Article Description (US Import)	General Rate	Special Rate	Rate2	Comments
CCC1O(CCCO)(CCC1O)CC		2912.50.0000	<ul style="list-style-type: none">- Aldehydes, whether or not with other oxygen function, cyclic polymers of aldehydes; paraformaldehyde;- Cyclic polymers of aldehydes;- Other	0.5%	Free (US, EU, CN, CL, CO, D, E, J, K, L, MA, MX, OM, PH, I)	40%	*** 25% ADDITIONAL TARIFFS IF COO IS CHINA AND NO USHTS EXEMPTION ***

Solving the challenge of Chapter 29

The challenge of Chapter 29 has always been its complexity, depth and detail. Even experienced chemists rarely achieve more than 50% accuracy when given the task.

In many organisations, the job of obtaining a HS code is often given to trade compliance departments, which typically have little to no chemical knowledge. In these circumstances, errors aren't avoidable; they're inevitable.

Built by scientists, for both chemists and non-chemists, ExpediChem is a simple and easy-to-use web-based platform that can quickly and accurately achieve high-quality HS and duty determinations for commercial and proprietary chemicals. It can process large chemical libraries running into millions of substances while still delivering highly accurate results.

ExpediChem is a comprehensive rule-based computational system. There are no gaps in knowledge, personal preferences or subjectivity. Decisions are clear, consistent and non-subjective.

This intelligent and intuitive software can be used by anyone, without the need for detailed knowledge of HTS schedules. Its low-cost makes it an attractive tool for any chemical company. Codes can be generated automatically and validated manually for total confidence in their accuracy.

Chapter 29 coding errors have the potential to cost your business hundreds of thousands of dollars every year in unnecessary taxes. If you're confident your chemical is covered by Chapter 29, ExpediChem is the fastest, cheapest and most accurate way to code it.

It's the single solution to the challenge of Chapter 29.



“This intelligent and intuitive software can be used by anyone, without the need for detailed knowledge of HTS schedules”



Business benefits

ExpediChem can help your business to save time and money by automating the HS code identification process. Here's how...



Faster coding, bigger savings

In business, time is money. ExpediChem can provide a highly accurate HS code in seconds, as opposed to hours, days or weeks. This can generate significant process and efficiency savings.



Cutting consultant costs

A subscription to ExpediChem is much cheaper than trade compliance lawyers or chemical consultants who can charge up to \$800 per hour. Automated HS coding enables you to use your business's resources more effectively by working more efficiently.



Tackling taxes

ExpediChem can have a dramatic impact on your tax liability, potentially saving you tens of thousands of dollars every year.

EXAMPLE ONE

Here's an example of how ExpediChem can help you save money. A company has a shipment of 500 chemicals with a value of \$250,000 to export. They're unable to manually code this amount of chemicals in a reasonable timeframe so declare them with a general chemicals HS code with the highest duty rate of 6.5% to prevent the risk of accidental tax fraud.

In this case, the total duty to be paid is \$16,250.

Using ExpediChem, the business can generate accurate HS codes, which reflect the exact liability due – which in many cases, is much lower. In this example, the exact duty is \$13,812.

A saving of \$2,438 for a single shipment.

EXAMPLE TWO

In another example, four proprietary compounds were custom synthesised and shipped to a customer on the gram scale for \$142,000. The duty was manually determined by the synthesising chemist to be 4.8% based on the structures of the compounds. However, the chemist had missed some essential parts buried in the hundreds of pages of HS regulations, additional explanatory notes and country-specific rules which accurately classified the duty rate as 0%.

Scitegrity's ExpediChem platform saved \$6,815 for a single shipment.

About Scitegrity

For more information on ExpediChem,
[visit \[www.scitegrity.com\]\(http://www.scitegrity.com\)](http://www.scitegrity.com)

Founded in 2011 by former pharmaceutical scientists, chemists and data managers, Scitegrity specialises in allowing the searching of chemical regulations.

Our software solutions are relied on by dozens of chemical and pharmaceutical companies, CROs and regulators globally, including half of the world's top-10 pharmaceutical companies.

Scitegrity also provides other related chemical legislation compliance services, such as Controlled Substances Squared for the automatic identification of controlled and regulated substances including Ozone Depleting, Controlled Drugs, Chemical Weapons, Military Dual-Use Lists, ITAR, CCL and other chemical regulations.



System coverage and limitations

We are developing the capacity and potential for ExpediChem all the time, adding new functionality and improvements to the system.

ExpediChem covers Chapter 29 of the HTSUS, Schedule B, EU and Chinese tariff schedules and includes the Pharmaceutical Appendix and the Chemical Appendix (applicable to the US only). However, it does not handle inorganics, composites, polymers or biologics (which are not part of Chapter 29).

Some Chapter 29 sub-headings use vague and ill-defined terminology. For example, sub-heading 2937 (provitamins, vitamins and hormones) carries a note relating to hormones which reads:

"...hormone derivatives and structural analogues used primarily for their hormonal effect, but also to those derivatives and structural analogues used primarily as intermediates in the synthesis of products of this heading".

Derivatives and analogues are nebulous terms with no clear or agreed chemical boundaries or definitions. This is a problem for both manual and automated assessments. For these areas, if the user indicates it's a hormone, the system will attempt to use substructure and similarity searching to determine if the substance is similar to any of the hormone classes listed in the chapter sub-headings.

The final limitation is the 'essential character' problem of the product. Take, for example, acetic acid (more widely known as the main ingredient of vinegar). This is classified as 2915 within Chapter 29. However, if it is below 10% by weight in solution, it is better placed under Chapter 22 – Beverages, Spirits and Vinegar, as its 'essential character' is that of table vinegar.

Despite these limitations, for the vast majority of organic chemicals, ExpediChem can achieve highly accurate determinations.

Endnotes

- 1 Evaluation of the European Customs Inventory of Chemical Substance (ECICS). <https://op.europa.eu/en/publication-detail/-/publication/cfc3556a-e46e-11e7-9749-01aa75ed71a1/language-en/format-PDF/source-55745419>.
- 2 ECICS (https://ec.europa.eu/taxation_customs/dds2/ecics/chemicalsubstance_consultation.jsp?Lang=en) The European Customs Inventory for Chemical Substances (ECICS), a publicly available database of non-binding, manually assigned HS/CN number from the EU Taxation and Customs Directorate General.
- 3 Pubchem (<https://pubchem.ncbi.nlm.nih.gov/>) is a publicly available database of chemicals maintained by the National Institutes of Health.
- 4 CROSS (<https://rulings.cbp.gov/home>). Allows a text-based search for US Customs rulings (all chapters) and submission of specific queries.

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